Davide Donadio

List of Publications by Year
in descending order

149 papers	21,746 citations	41258 49 h-index	9553 142 g-index
154 all docs	154 docs citations	154 times ranked	24394 citing authors

#	Article	IF	Citations
1	Canonical sampling through velocity rescaling. Journal of Chemical Physics, 2007, 126, 014101.	1.2	11,867
2	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	3.0	1,448
3	Length-dependent thermal conductivity in suspended single-layer graphene. Nature Communications, 2014, 5, 3689.	5.8	735
4	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	9.0	655
5	Atomistic Simulations of Heat Transport in Silicon Nanowires. Physical Review Letters, 2009, 102, 195901.	2.9	251
6	Freezing of a Lennard-Jones Fluid: From Nucleation to Spinodal Regime. Physical Review Letters, 2006, 97, 105701.	2.9	227
7	Homogeneous ice nucleation from supercooled water. Physical Chemistry Chemical Physics, 2011, 13, 19807.	1.3	226
8	Force and heat current formulas for many-body potentials in molecular dynamics simulations with applications to thermal conductivity calculations. Physical Review B, 2015, 92, .	1.1	215
9	Metadynamics Simulations of the High-Pressure Phases of Silicon Employing a High-Dimensional Neural Network Potential. Physical Review Letters, 2008, 100, 185501.	2.9	207
10	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. Nature Materials, 2006, 5, 623-626.	13.3	198
11	Thermal Conductivity of Isolated and Interacting Carbon Nanotubes: Comparing Results from Molecular Dynamics and the Boltzmann Transport Equation. Physical Review Letters, 2007, 99, 255502.	2.9	171
12	Blocking Phonon Transport by Structural Resonances in Alloy-Based Nanophononic Metamaterials Leads to Ultralow Thermal Conductivity. Physical Review Letters, 2016, 117, 025503.	2.9	153
13	Nanophononics: state of the art and perspectives. European Physical Journal B, 2016, 89, 1.	0.6	149
14	Temperature Dependence of the Thermal Conductivity of Thin Silicon Nanowires. Nano Letters, 2010, 10, 847-851.	4.5	146
15	Hamiltonian Adaptive Resolution Simulation for Molecular Liquids. Physical Review Letters, 2013, 110, 108301.	2.9	145
16	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 1443-1449.	2.3	139
17	Divergence of the thermal conductivity in uniaxially strained graphene. Physical Review B, 2013, 87, .	1.1	131
18	Experimental and theoretical evidence for bilayer-by-bilayer surface melting of crystalline ice. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 227-232.	3.3	131

#	Article	IF	Citations
19	Influence of thermostatting on nonequilibrium molecular dynamics simulations of heat conduction in solids. Journal of Chemical Physics, 2019, 151, 234105.	1.2	126
20	Thermal Transport in Nanoporous Silicon: Interplay between Disorder at Mesoscopic and Atomic Scales. ACS Nano, 2011, 5, 1839-1844.	7.3	122
21	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. Nature Communications, 2019, 10, 3853.	5.8	122
22	Highly anisotropic thermal conductivity of arsenene: Anab initiostudy. Physical Review B, 2016, 93, .	1.1	114
23	Thermal conductivity decomposition in two-dimensional materials: Application to graphene. Physical Review B, 2017, 95, .	1.1	113
24	Ice nucleation at the nanoscale probes no manâ€™s land of water. Nature Communications, 2013, 4, 1887.	5.8	112
25	Lattice thermal conductivity of semiconducting bulk materials: atomistic simulations. Physical Chemistry Chemical Physics, 2012, 14, 16209.	1.3	111
26	Heat transport in amorphous silicon: Interplay between morphology and disorder. Applied Physics Letters, 2011, 98, .	1.5	110
27	Hyperbranched Unsaturated Polyphosphates as a Protective Matrix for Long-Term Photon Upconversion in Air. Journal of the American Chemical Society, 2014, 136, 11057-11064.	6.6	109
28	An electrochemical thermal transistor. Nature Communications, 2018, 9, 4510.	5.8	105
29	Tuning Thermal Transport in Ultrathin Silicon Membranes by Surface Nanoscale Engineering. ACS Nano, 2015, 9, 3820-3828.	7.3	104
30	Dehydroxylation and Silanization of the Surfaces of Î²-Cristobalite Silica:Â An ab Initio Simulation. Journal of Physical Chemistry B, 2001, 105, 8007-8013.	1.2	95
31	Polyamorphism of Ice at Low Temperatures from Constant-Pressure Simulations. Physical Review Letters, 2004, 92, 225702.	2.9	93
32	Surface-induced crystallization in supercooled tetrahedral liquids. Nature Materials, 2009, 8, 726-730.	13.3	84
33	Growth of Nanostructured Carbon Films by Cluster Assembly. Physical Review Letters, 1999, 83, 776-779.	2.9	82
34	Evolution of the structure of amorphous ice: From low-density amorphous through high-density amorphous to very high-density amorphous ice. Journal of Chemical Physics, 2005, 122, 134501.	1.2	77
35	Microscopic Mechanism and Kinetics of Ice Formation at Complex Interfaces: Zooming in on Kaolinite. Journal of Physical Chemistry Letters, 2016, 7, 2350-2355.	2.1	77
36	Thermal transport in phase-change materials from atomistic simulations. Physical Review B, 2012, 86, .	1.1	75

#	Article	IF	Citations
37	Stability of hydrocarbons at deep Earth pressures and temperatures. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6843-6846.	3.3	72
38	Particle Formation in the Emulsionâ€Solvent Evaporation Process. Small, 2013, 9, 3514-3522.	5.2	71
39	Pressureâ€induced phase transitions in silicon studied by neural networkâ€based metadynamics simulations. Physica Status Solidi (B): Basic Research, 2008, 245, 2618-2629.	0.7	68
40	â€œSite Bindingâ€•of Ca2+Ions to Polyacrylates in Water:Â A Molecular Dynamics Study of Coiling and Aggregation. Macromolecules, 2007, 40, 3437-3442.	2.2	67
41	Monte Carlo Adaptive Resolution Simulation of Multicomponent Molecular Liquids. Physical Review Letters, 2013, 111, 060601.	2.9	67
42	Topological Defects and Bulk Melting of Hexagonal Ice. Journal of Physical Chemistry B, 2005, 109, 5421-5424.	1.2	66
43	Molecular Dynamics Study of the Solvation of Calcium Carbonate in Water. Journal of Physical Chemistry B, 2007, 111, 12219-12227.	1.2	66
44	Ab InitioSimulations of Photoinduced Interconversions of Oxygen Deficient Centers in Amorphous Silica. Physical Review Letters, 2001, 87, 195504.	2.9	63
45	Quasi-Ballistic Thermal Transport Across MoS₂ Thin Films. Nano Letters, 2019, 19, 2434-2442.	4.5	61
46	Autocatalytic and Cooperatively Stabilized Dissociation of Water on a Stepped Platinum Surface. Journal of the American Chemical Society, 2012, 134, 19217-19222.	6.6	53
47	Native surface oxide turns alloyed silicon membranes into nanophononic metamaterials with ultralow thermal conductivity. Physical Review B, 2017, 95, .	1.1	53
48	Direct observation of ultrafast hydrogen bond strengthening in liquid water. Nature, 2021, 596, 531-535.	13.7	53
49	Morphology and Temperature Dependence of the Thermal Conductivity of Nanoporous SiGe. Nano Letters, 2011, 11, 3608-3611.	4.5	51
50	Statistical mechanics of Hamiltonian adaptive resolution simulations. Journal of Chemical Physics, 2015, 142, 064115.	1.2	49
51	Mechanical Tuning of Thermal Transport in a Molecular Junction. Journal of Physical Chemistry C, 2015, 119, 24636-24642.	1.5	49
52	Dimensionality and heat transport in Si-Ge superlattices. Applied Physics Letters, 2013, 102, .	1.5	47
53	A Strategy to Suppress Phonon Transport in Molecular Junctions Using Ï€-Stacked Systems. Journal of Physical Chemistry C, 2017, 121, 7175-7182.	1.5	47
54	From four- to six-coordinated silica: Transformation pathways from metadynamics. Physical Review B, 2007, 76, .	1.1	45

#	Article	IF	Citations
55	First-Principle Analysis of the IR Stretching Band of Liquid Water. Journal of Physical Chemistry Letters, 2010, 1, 1398-1402.	2.1	45
56	High Seebeck Coefficient and Unusually Low Thermal Conductivity Near Ambient Temperatures in Layered Compound Yb_{2â€“x}Eu_xCdSb₂. Chemistry of Materials, 2018, 30, 484-493.	3.2	45
57	DFT Research on the Dehydroxylation Reaction of Pyrophyllite 1. First-Principle Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 7051-7060.	1.2	43
58	Nuclear Quantum Effects in Water: A Multiscale Study. Journal of Chemical Theory and Computation, 2014, 10, 816-824.	2.3	42
59	Interaction of Charged Amino-Acid Side Chains with Ions: An Optimization Strategy for Classical Force Fields. Journal of Physical Chemistry B, 2014, 118, 3960-3972.	1.2	41
60	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. Journal of Applied Physics, 2015, 117, .	1.1	41
61	Toward Hamiltonian Adaptive QM/MM: Accurate Solvent Structures Using Many-Body Potentials. Journal of Chemical Theory and Computation, 2016, 12, 3441-3448.	2.3	41
62	Photoelasticity of sodium silicate glass from first principles. Physical Review B, 2004, 70, .	1.1	39
63	Influence of Temperature and Anisotropic Pressure on the Phase Transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Cristobalite. Physical Review Letters, 2008, 100, 165502.	2.9	38
64	Structure and Dynamics of the Quasi-Liquid Layer at the Surface of Ice from Molecular Simulations. Journal of Physical Chemistry C, 2018, 122, 24780-24787.	1.5	38
65	Combined Experimental and Theoretical Investigation of Heating Rate on Growth of Iron Oxide Nanoparticles. Chemistry of Materials, 2017, 29, 9648-9656.	3.2	37
66	Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP. Advanced Functional Materials, 2019, 29, 1900233.	7.8	37
67	Nucleation of tetrahedral solids: A molecular dynamics study of supercooled liquid silicon. Journal of Chemical Physics, 2009, 131, 224519.	1.2	34
68	Decisive role of nuclear quantum effects on surface mediated water dissociation at finite temperature. Journal of Chemical Physics, 2018, 148, 102320.	1.2	32
69	Photoelasticity of crystalline and amorphous silica from first principles. Physical Review B, 2003, 68, .	1.1	31
70	Cluster expansion and optimization of thermal conductivity in SiGe nanowires. Physical Review B, 2010, 81, .	1.1	31
71	Strongly tunable anisotropic thermal transport in MoS ₂ by strain and lithium intercalation: first-principles calculations. 2D Materials, 2019, 6, 025033.	2.0	31
72	Probing Properties of Water under Confinement: Infrared Spectra. Nano Letters, 2008, 8, 2959-2962.	4.5	30

#	Article	IF	Citations
73	Electronic Effects in the IR Spectrum of Water under Confinement. Journal of Physical Chemistry B, 2009, 113, 4170-4175.	1.2	30
74	Ab initioinvestigation of the melting line of nitrogen at high pressure. Physical Review B, 2010, 82, .	1.1	29
75	Thermal conductivity of one-, two- and three-dimensional sp²carbon. New Journal of Physics, 2013, 15, 105019.	1.2	29
76	A unified framework for force-based and energy-based adaptive resolution simulations. Europhysics Letters, 2014, 108, 30007.	0.7	29
77	Bimodal Grain-Size Scaling of Thermal Transport in Polycrystalline Graphene from Large-Scale Molecular Dynamics Simulations. Nano Letters, 2017, 17, 5919-5924.	4.5	28
78	Structural Complexity and High Thermoelectric Performance of the Zintl Phase: Yb₂₁Mn₄Sb₁₈. Chemistry of Materials, 2019, 31, 8076-8086.	3.2	28
79	Adsorption of Dichlorobenzene on Au and Pt Stepped Surfaces Using van der Waals Density Functional Theory. Journal of Physical Chemistry C, 2012, 116, 20409-20416.	1.5	27
80	Trends in the Adsorption and Dissociation of Water Clusters on Flat and Stepped Metallic Surfaces. Journal of Physical Chemistry C, 2014, 118, 29990-29998.	1.5	27
81	Thermal transport in free-standing silicon membranes: influence of dimensional reduction and surface nanostructures. European Physical Journal B, 2015, 88, 1.	0.6	27
82	IIIâ€“V Clathrate Semiconductors with Outstanding Hole Mobility: Cs8In27Sb19 and A8Ga27Sb19 (A = Cs,) Tj ETQq0 0 0 rgBT /Overlock	6.6	27
83	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of MnxGey compounds. Journal of Applied Physics, 2020, 127, .	1.1	27
84	Efficient anharmonic lattice dynamics calculations of thermal transport in crystalline and disordered solids. Journal of Applied Physics, 2020, 128, .	1.1	22
85	Tuning the Adsorption of Aromatic Molecules on Platinum via Halogenation. Journal of Physical Chemistry C, 2014, 118, 6235-6241.	1.5	21
86	Effect of van der Waals interactions on the chemisorption and physisorption of phenol and phenoxy on metal surfaces. Journal of Chemical Physics, 2016, 145, 104701.	1.2	21
87	Enhanced thermoelectric performance of two dimensional MS2 (MÂ=ÂMo, W) through phase engineering. Journal of Materiomics, 2018, 4, 329-337.	2.8	21
88	Ab initiosimulation of photoinduced transformation of small rings in amorphous silica. Physical Review B, 2005, 71, .	1.1	20
89	From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3030-3039.	2.3	20
90	Efficient thermal diode with ballistic spacer. Physical Review E, 2018, 97, 030101.	0.8	20

#	Article	IF	Citations
91	Atomistic simulations of thermal conductivity in GeTe nanowires. Journal Physics D: Applied Physics, 2020, 53, 054001.	1.3	20
92	Simulating Energy Relaxation in Pumpâ€“Probe Vibrational Spectroscopy of Hydrogen-Bonded Liquids. Journal of Chemical Theory and Computation, 2017, 13, 1284-1292.	2.3	18
93	Ultrahigh Convergent Thermal Conductivity of Carbon Nanotubes from Comprehensive Atomistic Modeling. Physical Review Letters, 2021, 127, 025902.	2.9	18
94	DFT Research on the Dehydroxylation Reaction of Pyrophyllite 2. Characterization of Reactants, Intermediates, And Transition States along the Reaction Path. Journal of Physical Chemistry A, 2008, 112, 6373-6383.	1.1	17
95	Exploring the Rehydroxylation Reaction of Pyrophyllite by Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 7593-7601.	1.2	17
96	Atomistic calculation of the thermal conductance of large scale bulk-nanowire junctions. Physical Review B, 2011, 84, .	1.1	17
97	Accurate and general treatment of electrostatic interaction in Hamiltonian adaptive resolution simulations. European Physical Journal: Special Topics, 2016, 225, 1505-1526.	1.2	17
98	Hierarchical thermoelectrics: crystal grain boundaries as scalable phonon scatterers. Nanoscale, 2016, 8, 3729-3738.	2.8	17
99	Thermal transport in amorphous small organic materials: a mechanistic study. Physical Chemistry Chemical Physics, 2020, 22, 3058-3065.	1.3	16
100	Synergistic impeding of phonon transport through resonances and screw dislocations. Physical Review B, 2021, 103, .	1.1	16
101	Engineering Thermal Transport across Layered Grapheneâ€“MoS₂ Superlattices. ACS Nano, 2021, 15, 19503-19512.	7.3	16
102	Silicon stops heat in its tracks. Nature Nanotechnology, 2010, 5, 701-702.	15.6	15
103	Thermal transport across graphene step junctions. 2D Materials, 2019, 6, 011005.	2.0	15
104	Theoretical investigation of methane under pressure. Journal of Chemical Physics, 2009, 130, 164520.	1.2	14
105	Photodecay of guaiacol is faster in ice, and even more rapid on ice, than in aqueous solution. Environmental Sciences: Processes and Impacts, 2020, 22, 1666-1677.	1.7	14
106	Anisotropic In-Plane Phonon Transport in Silicon Membranes Guided by Nanoscale Surface Resonators. Physical Review Applied, 2020, 14, .	1.5	14
107	Bathochromic Shift in the UVâ€“Visible Absorption Spectra of Phenols at Ice Surfaces: Insights from First-Principles Calculations. Journal of Physical Chemistry A, 2020, 124, 9288-9298.	1.1	14
108	The interplay between surfaceâ€“water and hydrogen bonding in a water adlayer on Pt(111) and Ag(111). Journal of Physics Condensed Matter, 2007, 19, 242101.	0.7	13

#	Article	IF	Citations
109	Migration of positively charged defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz. Physical Review B, 2007, 76, .	1.1	13
110	Optimal thickness of silicon membranes to achieve maximum thermoelectric efficiency: A first principles study. Applied Physics Letters, 2016, 109, 053902.	1.5	13
111	Molecular Mechanism of Crystal Growth Inhibition at the Calcium Oxalate/Water Interfaces. Journal of Physical Chemistry C, 2016, 120, 4410-4417.	1.5	13
112	Atomistic simulations of heat transport in real-scale silicon nanowire devices. Applied Physics Letters, 2012, 100, .	1.5	12
113	Mode localization and suppressed heat transport in amorphous alloys. Physical Review B, 2021, 103, .	1.1	12
114	Effect of crystallinity and thickness on thermal transport in layered PtSe2. Npj 2D Materials and Applications, 2022, 6, .	3.9	12
115	Simulation of atomic force microscopy of fractal nanostructured carbon films. Europhysics Letters, 2001, 54, 72-76.	0.7	11
116	Dissociative Adsorption of Water at (211) Stepped Metallic Surfaces by First-Principles Simulations. Journal of Physical Chemistry C, 2017, 121, 16783-16791.	1.5	11
117	Solid Solution Yb2â€“xCaxCdSb2: Structure, Thermoelectric Properties, and Quality Factor. Inorganic Chemistry, 2021, 60, 13596-13606.	1.9	11
118	Energy Relaxation and Thermal Diffusion in Infrared Pumpâ€“Probe Spectroscopy of Hydrogen-Bonded Liquids. Journal of Physical Chemistry Letters, 2019, 10, 3447-3452.	2.1	10
119	Carbon dioxide, bicarbonate and carbonate ions in aqueous solutions under deep Earth conditions. Physical Chemistry Chemical Physics, 2020, 22, 10717-10725.	1.3	10
120	Proton Wires via One-Dimensional Water Chains Adsorbed on Metallic Steps. Journal of Chemical Theory and Computation, 2011, 7, 2681-2684.	2.3	9
121	Molecular simulation of oligo-glutamates in a calcium-rich aqueous solution: insights into peptide-induced polymorph selection. CrystEngComm, 2015, 17, 6863-6867.	1.3	9
122	Beating the Thermal Conductivity Alloy Limit Using Long-Period Compositionally Graded Si_{1â€“x}Ge_x Superlattices. Journal of Physical Chemistry C, 2020, 124, 19864-19872.	1.5	9
123	Elastic moduli of nanostructured carbon films. Physical Review B, 2004, 70, .	1.1	7
124	Non-equilibrium dynamics and structure of interfacial ice. Chemical Physics Letters, 2006, 426, 115-119.	1.2	7
125	Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations. Journal of Physical Chemistry C, 2013, 117, 7526-7532.	1.5	7
126	Practical algorithms to facilitate large-scale first-principles molecular dynamics. Journal of Physics: Conference Series, 2009, 180, 012074.	0.3	6

#	Article	IF	Citations
127	Adsorption of polyiodobenzene molecules on the Pt(111) surface using van der Waals density functional theory. Surface Science, 2016, 644, 113-121.	0.8	6
128	Nanofriction Behavior of Cluster-Assembled Carbon Films. Journal of Nanoscience and Nanotechnology, 2002, 2, 637-643.	0.9	5
129	Freezing point depression in model Lennard-Jones solutions. Molecular Physics, 2015, 113, 2725-2734.	0.8	5
130	Advances in the optimization of silicon-based thermoelectrics: a theory perspective. Current Opinion in Green and Sustainable Chemistry, 2019, 17, 35-41.	3.2	5
131	Mn-intercalated MoSe2 under pressure: Electronic structure and vibrational characterization of a dilute magnetic semiconductor. Journal of Chemical Physics, 2020, 153, 124701.	1.2	5
132	Enhanced photodegradation of dimethoxybenzene isomers in/on ice compared to in aqueous solution. Atmospheric Chemistry and Physics, 2022, 22, 5943-5959.	1.9	5
133	Simulation of the grafting of organosilanes at the surface of dry amorphous silica. Journal of Physics Condensed Matter, 2008, 20, 224011.	0.7	4
134	Covalent Cluster-Assembled Carbon Solids. , 2001, , 89-126.		4
135	Atomic scale characterization of nanostructured a-C:H films. European Physical Journal B, 2002, 27, 335-340.	0.6	3
136	Ab initiocharacterization of graphene nanoribbons and their polymer precursors. Journal of Physics Condensed Matter, 2012, 24, 104023.	0.7	3
137	Simulation of Dimensionality Effects in Thermal Transport. Lecture Notes in Physics, 2016, , 275-304.	0.3	3
138	Selective adsorption of a supramolecular structure on flat and stepped gold surfaces. Surface Science, 2018, 670, 44-50.	0.8	3
139	Unprecedented superstructure in the type I family of clathrates. Chemical Communications, 2021, 57, 13780-13783.	2.2	3
140	Thermal Transport: Overview. , 2018, , 1-11.		2
141	PbTe/PbSe Thermoelectric Nanocomposites: The Impact of Length Modulations on Lowering Thermal Conductivity. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	0.6	2
142	Evolution of structure and transport properties of the Ba8Cu16P30 clathrate-I framework with the introduction of Ga. Applied Physics Letters, 2022, 120, .	1.5	2
143	Barbalinardo etÂal. Reply:. Physical Review Letters, 2022, 128, .	2.9	2
144	Thermal transport in finite-size van der Waals materials: Modeling and Simulations. , 2018, , .		1

#	Article	IF	Citations
145	Nanofriction behavior of cluster-assembled carbon films. Journal of Nanoscience and Nanotechnology, 2002, 2, 637-43.	0.9	1
146	Hybrid Materials: Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP (Adv. Funct. Mater. 18/2019). Advanced Functional Materials, 2019, 29, 1970120.	7.8	0
147	Evolution of the structure of amorphous ice - from LDA through HDA to VHDA. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c87-c87.	0.3	0
148	Stability of hydrocarbons at deep Earth pressures and temperatures. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C168-C168.	0.3	0
149	Thermal Transport: Overview. , 2020, , 723-733.		0